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CONCURRENT MICROMECHANICAL TAILORING AND FABRICATION PROCESS OPTIMIZATION FOR METAL-MATRIX COMPOSITES

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ABSTRACT

A method is presented to minimize the residual matrix stresses in metal matrix composites. Fabrication parameters such as temperature and consolidation pressure are optimized concurrently with the characteristics (ie., modulus, coefficient of thermal expansion, strength, and interphase thickness) of a fiber-matrix interphase. By including the interphase properties in the optimization of the fabrication process, lower residual stresses are achievable. Results for a ultra-high modulus graphite (P100)/copper composite show a reduction of 21% for the maximum matrix microstress when optimizing the fabrication process alone. Concurrent optimization of the fabrication process and interphase properties show a 41% decrease in the maximum microstress. Therefore, this optimization method demonstrates the capability of reducing residual microstresses by altering the temperature and consolidation pressure histories and tailoring the interphase properties for an improved composite material. In addition, the results indicate that the consolidation pressures are the most important fabrication parameters, and the coefficient of thermal expansion is the most critical interphase property.

NOMENCLATURE

d_f	Fiber diameter.
E	Young's Modulus.
$F(z)$	Objective function.

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G	Shear Modulus.
$Q(z)$	Inequality constraint.
k_d	Interphase thickness.
k_f	Fiber volume ratio.
P	Property.
p	Pressure.
S	Ultimate Strength.
T	Temperature.
T_M	Melting temperature.
t	Time.
w	Weight coefficient.
z	Optimization Parameter.
α	Thermal expansion coefficient.
ρ	Mass Density.
σ	Stress or Microstress.
ν	Poisson's ratio.

Superscripts

C	Compression.
L	Lower bound.
T	Tension.
U	Upper bound.

Subscripts

d	Interphase.
f	Fiber.
m	Matrix.
l	Composite.
n	Normal.
o	Reference.
s	Shear.
$1, 2, 3$	Composite material coordinate system axes.

1. INTRODUCTION

Metal-matrix composites (MMC) have generated a high-degree of interest for aerospace and structural applications. Despite their high cost, MMCs are potential candidates for specific applications demanding high operational temperatures (from 400°C to 1100°C), hygrothermal resistance, stability, and peak mechanical performance. A crucial problem limiting the use of many MMCs is the high residual (final) thermal microstresses developed during the fabrication process, as a result of the large temperature differential and the mismatch between the thermal expansion coefficients (CTE) of the fiber and matrix. The presence of residual microstresses typically degrades the mechanical performance of the composite and is primarily responsible for the reported poor thermo-mechanical fatigue endurance of many MMCs.

It is desirable, therefore, to explore possible ways to reduce, or alternatively control, the development of residual microstresses. One possibility is to use a suitable fiber coating as an interphase layer between the fibers and the matrix to reduce the effects of the fiber/matrix CTE mismatch [1]. Recent work [2] has also shown that reductions in residual stresses may be also attained with optimal combinations of temperature and consolidation pressure during fabrication. Hence, it seems advantageous to tailor not only the interphase properties, but also the temperature and consolidation pressure profiles of the fabrication process concurrently to achieve acceptable residual microstresses.

This paper presents the development of methodologies for: (1) the simulation of the micromechanical nonlinear response of unidirectional MMCs with three material phases (fiber, matrix, and interphase) during fabrication; and (2) the concurrent tailoring of the interphase layer with optimal fabrication considerations. The objective is to minimize the residual matrix microstresses at the end of the fabrication process by optimizing the temperature and consolidation pressure histories concurrently with the interphase properties (modulus, CTE, strength) and other composite parameters (interphase thickness and fiber volume ratio (FVR)), while the material integrity throughout the process is ensured. By concurrently optimizing the process and the interphase, greater

reductions in residual microstresses are achieved when compared to individual optimization of the interphase and fabrication process. Finally, applications of this method are shown for an ultra-high modulus graphite (P100)/copper composite system.

2. FABRICATION PROCESS

A typical fabrication cycle, as the one shown in Fig. 1 for P100/copper, usually involves three phases. During Phase 1 the temperature of the raw materials (rows of fibers stacked between ultra-thin foils of matrix, or rows of fibers in metallic powder, or tows of graphite fibers preimpregnated in the metallic matrix by the chemical vapor deposition method) is elevated near the matrix melting point. Usually, the maximum temperature remains lower than the melting temperature of the matrix to reduce chemical reactions at the fiber-matrix interphase and matrix oxidation, which requires the application of higher consolidation pressure (Phase 2) such that the matrix is diffused and bonded with the fibers (superplastic diffusion bonding). Phase 2 is assumed sufficiently long, such that perfect bonding is accomplished and pre-existing residual stresses in the matrix are relaxed. In the final cool-down phase of the composite (Phase 3) the temperature and consolidation pressure are reduced to room conditions.

Phase 3 is the more critical phase of the fabrication process because significant residual microstresses are developed in the matrix and the fibers, as a result of the mismatch between the CTE of the fibers and matrix. Mechanical microstresses are also present during phase 3 as a result of the consolidation pressure, but they vanish at the end of the fabrication when the consolidation pressure is removed. Since the build-up of residual stresses and the integrity of the composite material are primarily affected by the temperature and consolidation pressure histories during Phase 3, it is reasonable to focus the current study on this stage of fabrication.

3. THERMO-MECHANICAL RESPONSE

The thermo-mechanical response of MMCs during Phase 3 of the fabrication process was based on a unified non-linear micromechanics theory developed by Chamis and coworkers [3-5]. The theory incorporates, among other factors, three material phases (fiber, matrix, and interphase), temperature effects, and mechanical non-linearities. An in-house

code (METCAN: METal-matrix Composite ANalyzer) was used to simulate the thermo-mechanical response of the MMCs. The basic elements of the method are summarized in this section.

The micromechanics theory assumes the composite microstructure shown in Fig. 2 consisting of three material phases: the fiber (f), the matrix (m) , and an interphase (d). In this paper the interphase represents the fiber coating placed between the fiber and the matrix to reduce the build-up of thermal residual stresses in the matrix. Three distinct micro-regions are recognized in the composite material [5], as shown in Fig. 2, which are identified with subscripts A (matrix), B (matrix-interphase), and C (matrix-interphase-fibers). Micro-regions A, B, and C have different average properties, therefore, mechanical or thermal loads result in the development of different average stresses.

The average properties of the composite, as well as, the average properties of microregions A, B, and C are provided as explicit functions of the properties and the volume ratios (k) of the three constituents. In general,

$$P_j^t = f(P_m^t, P_d^t, P_f^t, k_f, k_d) \qquad j = l, A, B, C \tag{1}$$

where P represents a specific property and subscript j represents either the composite (l) or microregions A, B, and C. Subscripts m, d, and f identify the matrix, interphase and fiber respectively, and superscript t properties at time t. The theory assumes constant average stresses in each microregion, admissible boundary conditions, and equilibrium of stresses. The assumption of constant average stress mandates the correction of the fiber and interphase volume ratios in the transverse and shear directions. The latter assumption has been extensively applied in the development of micromechanics for polymer composites, and has provided good accuracy at minimal computational cost.

In the present paper the nonlinear effects of state variables, such as temperature and stress, on the in situ properties of the constituent materials are represented by the following form:

$$\frac{P_i^t}{P_{oi}} = [\frac{T_{Mi} - T^t}{T_{Mi} - T_o}]^q [\frac{S_i^t - \sigma_i^t}{S_i^t}]^p \qquad i = m, d, f \tag{2}$$

where: subscript i indicates matrix, interphase, or fibers; subscript o reference conditions; subscript M the melting point. Candidate properties for this equation are the moduli

(E), Poisson's ratios(ν), strengths (S), and CTE (α) of the constituents. The first term in the right hand side of eq. 2 represents the temperature effects and the second term the mechanical nonlinearity in a stress-strain curve. Time effects have been neglected. All exponents in eq. 2 are estimated from correlations with experimental data.

Because of the non-linear behavior of the material, an incremental procedure was used. In this context, the mechanical composite stresses, the temperature, and the microstresses at time $t + \Delta t$ are from the respective cumulative quantities at time t and their increments during time step Δt, that is:

$$\{\sigma_l^{t+\Delta t}\} = \{\sigma_l^t\} + \{\sigma_l\} \tag{3.1}$$

$$T^{t+\Delta t} = T^t + T \tag{3.2}$$

$$\{\sigma_j^{t+\Delta t}\} = \{\sigma_j^t\} + \{\sigma_j\} \tag{3.3}$$

where time superscripts and no superscripts indicate cumulative and incremental quantities respectively. The subscript j represents each microregion.

The incremental microstresses in eq. 3.3 at the different regions of the composite induced by the incremental stresses $\{\sigma_l\}$ and temperature T, are calculated from closed-form expressions derived on the previously stated micromechanical assumptions and linear elastic response for the homogenized composite and the individual constituent materials during time step Δt.

$$\{\sigma_j\} = f(\{\sigma_l\}, T, P_j^t, P_l^t, k_f, k_d) \tag{4}$$

The properties of the constituent materials P_j^t in eq. 4 are calculated from eq. 2, and the equivalent composite properties P_l^t from eqs. 1-2. The highly nonlinear behavior of the matrix and the interphase requires either the use of sufficiently small time steps Δt, or combinations of larger time steps and an iterative procedure. The latter technique was used in the present paper.

4. FABRICATION/INTERPHASE OPTIMIZATION

The proposed method aims to minimize the residual matrix microstresses by optimizing: (1) the consolidation temperature and pressure, and (2) the mechanical characteristics of the interphase. Considering the large number of parameters and the complexity of the simulation, this may be best accomplished with non-linear mathematical programming (NLP). It is recalled that a standard constrained NLP problem involves the minimization of an objective function:

$$\min\ F(\mathbf{z}) \tag{5.1}$$

subject to constraints in the following form:

$$\mathbf{z}^{\mathbf{L}} \leq \mathbf{z} \leq \mathbf{z}^{\mathbf{U}} \tag{5.2}$$

$$Q(\mathbf{z}) \leq \mathbf{0} \tag{5.3}$$

In the present paper emphasis is placed on the minimization of the matrix stresses in region A. In the case of open-die consolidation (ie. application of equal pressure in both transverse directions 22 and 33, and no pressure in the longitudinal direction 11), only the normal microstresses σ_{mA11} and σ_{mA22}, (where $\sigma_{mA22} = \sigma_{mA33}$, exist in the matrix (region A). Among the many possible ways for these stresses to be minimized simultaneously, the mini-max formulation, ie. minimize the maximum stress, is proposed for its tendency to result in equal minimum stresses. Therefore, the optimal fabrication problem is first formulated as the following constrained optimization,

$$\min(\max\{w_1\sigma_{mA11}, w_2\sigma_{mA22}\}) \tag{6}$$

subject to upper and lower bounds (5.2) on the optimization vector $\mathbf{z}$. The optimization vector includes: (1) the temperatures, consolidation pressures, and times at n_p control points defining, $n_p - 1$ segments of linear temperature and pressure variations; and (2) critical mechanical properties of the candidate interphase in reference conditions, such as the modulus, ultimate strength, CTE, and so forth.

Constraints are also imposed on the matrix, interphase, and fiber microstresses at n_s time steps in the form of the maximum stress criterion,

$$(S^C_{mk11})_j < (\sigma_{mk11})_j < (S^T_{mk11})_j \qquad j = 1, ..., n_p \text{ and } k = A, B, C \tag{7.1}$$

$$(S^C_{mk22})_j < (\sigma_{mk22})_j < (S^T_{mk22})_j \qquad j = 1, ..., n_p \text{ and } k = A, B, C \tag{7.2}$$

$$(S^C_{dk11})_j < (\sigma_{dk11})_j < (S^T_{dk11})_j \qquad j = 1, ..., n_p \text{ and } k = B, C \tag{7.3}$$

$$(S^C_{dk22})_j < (\sigma_{dk22})_j < (S^T_{dk22})_j \qquad j = 1, ..., n_p \text{ and } k = B, C \tag{7.4}$$

$$(S^C_{fC11})_j < (\sigma_{fC11})_j < (S^T_{fC11})_j \qquad j = 1, ..., n_s \tag{7.5}$$

$$(S^C_{fC22})_j < (\sigma_{fC22})_j < (S^T_{fC22})_j \qquad j = 1, ..., n_p \tag{7.6}$$

The superscripts C and T identify compressive and tensile strengths respectively. An additional constraint is imposed on the interphase thickness t_d, to ensure topological compatibility in the case for square packing of fibers:

$$1 + \frac{2t_d}{d_f} - \sqrt{\frac{\pi}{4k_f}} \leq 0 \tag{7.7}$$

Whereas, d_f is the fiber diameter and k_f is the FVR.

The optimization criteria described by eqs. 6-7 are transformed to an equivalent NLP compatible formulation (eqs. 5) as follows:

$$\min(\zeta) \tag{8.1}$$

subject to constraints,

$$w_1 \sigma_{mA11} \leq \zeta \tag{8.2}$$

$$w_2 \sigma_{mA22} \leq \zeta \tag{8.3}$$

in addition to constraints (5.2) and (7). The objective function ζ is an additional design variable. The NLP problem described by eqs. 8, 5.2, and 7 is numerically solved with the modified feasible directions non-linear programming method [6]. The modified feasible directions algorithm performs a direct search within the feasible optimization domain. The search direction is estimated from first order sensitivity of the objective function and the active constraints. A line search follows along the calculated search direction. The implemented algorithm includes an active set strategy, ie., only the constraints near violation are included in the search, thus allowing the efficient handling of the large number of constraints defined by eqs. (7).

5. APPLICATION AND DISCUSSION

An ultra-high modulus graphite (P100)/copper unidirectional MMC was used to test the optimization method for the fabrication process and the concurrent optimization of the process and interphase properties. Representative constituent properties of the composite system at reference conditions (21^oC, 0 Pa) are shown in Table 1. The Materials Division of NASA Lewis Research Center provided the current fabrication process for the P100/copper. Only the cool-down phase of the fabrication process will be simulated during the optimization and thermo-mechanical response of the MMC. The development of residual stresses and the integrity of the composite material are primarily affected by the temperature and pressure histories at this phase. Initial interphase properties were assumed equivalent to the matrix properties. In addition to the material properties, the initial interphase thickness was 12% of the fiber diameter and the FVR of the composite system was 40%.

The cool-down phase was subdivided into four increments of linearly varying temperature and pressure. Stress constraints were imposed at five evenly spaced time intervals in each linear segment. In this manner, twenty constraints were introduced for each microstress inequality described in eq. 7 , and where the interphase was optimized one additional constraint on the thickness will be added. The weighing coefficients were: $w_1 = w_2 = 1$. The temperatures, pressures, and times at the starting and final points of the four linear segments were used as optimization parameters. The temperature at the beginning of the cool-down phase was held constant and equal to the respective temperature of the current processes, and the final pressure was set equal to zero. Shown below are the upper and lower bounds imposed on the optimization method in accordance with eq. 5.2.

Fabrication Process Parameters:

$$T_o \leq T \leq T_M \tag{9.1}$$

$$0 \leq p \leq 345MPa \tag{9.2}$$

$$10sec \leq t \leq 18000sec \tag{9.3}$$

Interphase Property:

$$34.6GPa \leq E_d \leq 220.8GPa \tag{9.4}$$

$$1.69cm/cm/^oC \leq \alpha_d \leq 67.8cm/cm/^oC \tag{9.5}$$

$$34.5MPa \leq S_d \leq 414.0MPa \tag{9.6}$$

Micromechanical Parameters:

$$0.05 \leq k_d \leq 0.15 \tag{9.7}$$

$$0.05 \leq k_f \leq 0.55 \tag{9.8}$$

Figure 3 shows the current and the optimum fabrication processes, Case 1 (the fabrication process optimized alone) and Case 2 (concurrent optimization of the fabrication process and interphase properties), for the P100/copper MMC. Both optimized processes, Cases 1 and 2, follow similar patterns during the cool-down phase. Compared to the current process, two significant differences exist that lead to the reduction of the final residual matrix microstresses. First the optimized temperature histories in Fig. 3a decrease more rapidly to room temperature and are held constant until the end of the processes; secondly as shown in Fig. 3b, the predicted optimal consolidation pressures gradually increase as the consolidation temperature drops, reaching significantly higher values than the pressure of the current process and finally dropping to zero.

More interestingly, the temperature drop takes place when the pressure is high, indicating that the thermal stresses are forced to develop when the matrix and interphase are highly nonlinear and near "plastic", hence high strains result in low stresses. The pressure is removed when the temperature reaches room values as it does not contribute further. This illustrates the importance of the consolidation pressure. Apparently the values of the consolidation pressure were limited by the current strength of the constituents, as indicated by the observed active constraints in eq. 7. Shown in Fig. 4 are the predicted buildups of microstresses σ_{mA11} and σ_{mA22}. The final (residual) microstress σ_{mA11} for Case 1 decreased by 21% compared to the respective microstress value of the current process, in comparison, Case 2 had a 41% reduction for σ_{mA11}. The additional reductions in Case 2 were attributed to the interphase optimization. Microstress σ_{mA22} of the Case 1 was

nearly equivalent to the current process, however, the final microstress σ_{mA22} decreased by 24% because of optimized interphase properties.

The optimization of the interphase properties between the fiber and matrix, refer to Fig. 2, resulted in an optimum interphase with compatible properties (Table 2) to the fabrication process and fiber. The fact that the initial interphase material was matrix indicates the need for an interphase between the fibers/matrix. As seen in Table 2, all interphase properties increased during the optimization. Specifically, the modulus and strength increased slightly, while the CTE had a larger increase. As indicated by the results, the CTE was the most critical interphase property. The interphase thickness and FVR also increased.

6. SUMMARY

A method was proposed for optimizing the fabrication process and interphase properties concurrently for unidirectional metal-matrix composites. The response of the fabricated MMC was simulated based on nonlinear micromechanics and the NLP problem was numerically solved with the modified feasible directions nonlinear programming method. Reduction in residual microstresses for the fabricated composite were optimized by varying temperature and pressure histories along with the interphase properties during the cool-down phase. An in-house research code has been developed incorporating this method.

Case studies were performed on ultra-high modulus graphite (P100)/copper composite. The predicted optimum process for the fabrication process reduced the maximum final microstress by 21%, by favorably optimizing the nonlinear in situ matrix behavior. By including the interphase properties in the optimization method a further reduction, 41%, in the final maximum microstress was achieved illustrating the importance of the interphase optimization. Finally, the results indicate that consolidation pressures are the most important fabrication parameters, and the CTE is the most critical interphase property.

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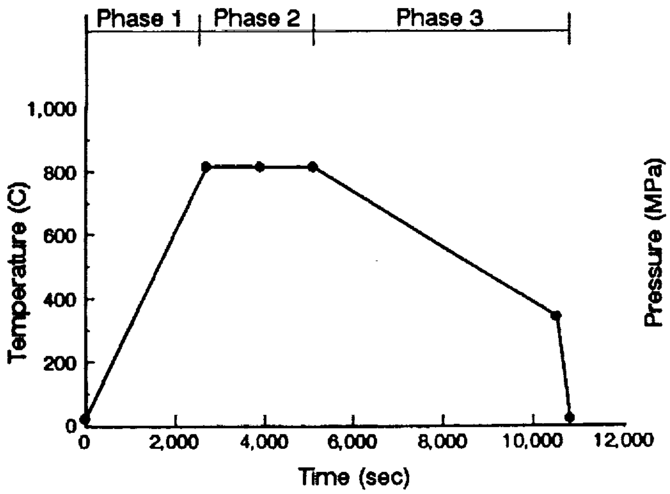
Table 1. Representative Constituent Mechanical Properties of P100/Copper at Reference Conditions.

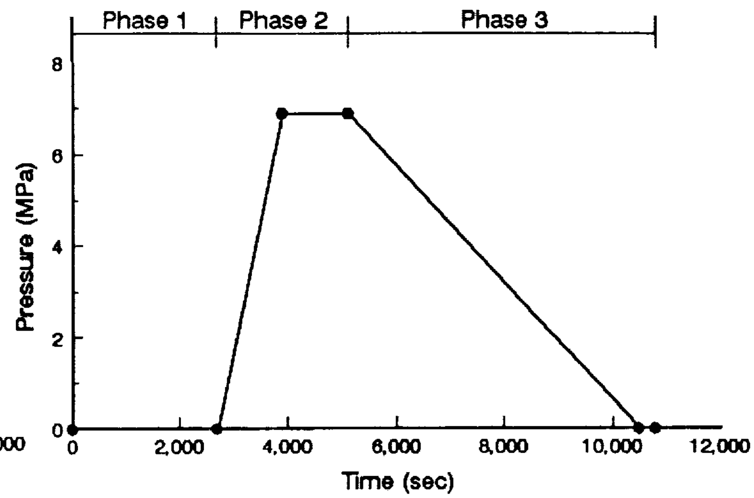
P100 Graphite	Copper
$E_{f11} = 105.0\ GPa$	$E_m = 122.1\ GPa$
$E_{f22} = 0.90\ GPa$	
$G_{f12} = 1.10\ GPa$	$G_m = 47.0\ GPa$
$G_{f23} = 0.70\ GPa$	
$\rho_f = 2.16\ g/cm^3$	$\rho_m = 8.86\ g/cm^3$
$\nu_{f12} = 0.20\ cm/cm$	$\nu_m = 0.30\ cm/cm$
$\nu_{f23} = 0.25\ cm/cm$	
$\alpha_{f11} = -0.030\ mcm/cm/^\circ C$	$\alpha_m = 0.331\ mcm/cm/^\circ C$
$\alpha_{f22} = 0.190\ mcm/cm/^\circ C$	
$S_{f11,T} = 2.242\ GPa$	$S_{mn} = 0.221\ GPa$
$S_{f11,C} = 1.380\ GPa$	
$S_{f22} = 0.1725\ GPa$	
$S_{f12} = 0.1725\ GPa$	$S_{ms} = 0.131\ GPa$
$S_{f23} = 0.0862\ GPa$	

Table 2. Initial and Optimized Interphase Properties for P100/Copper

Initial (Matrix)	Optimum
$E_d = 17.7\ Mpsi$	$E_d = 18.8\ Mpsi$
$\alpha_d = 9.80\ \mu in/in/^\circ F$	$\alpha_d = 15.0\ \mu in/in/^\circ F$
$S_d = 32.0\ ksi$	$S_d = 27.0\ ksi$
$k_d = 12\%$	$k_d = 15\%$
$k_f = 40\%$	$k_f = 47\%$



(a) Temperature



(b) Consolidation Pressure

Figure 1. - Typical Processing Cycle for Graphite/Copper Composite

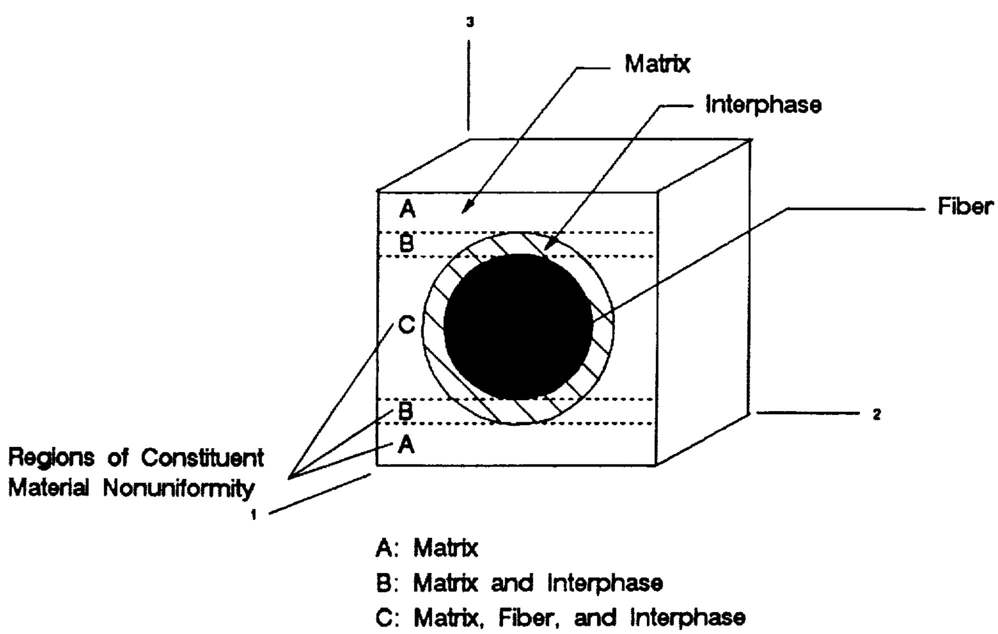
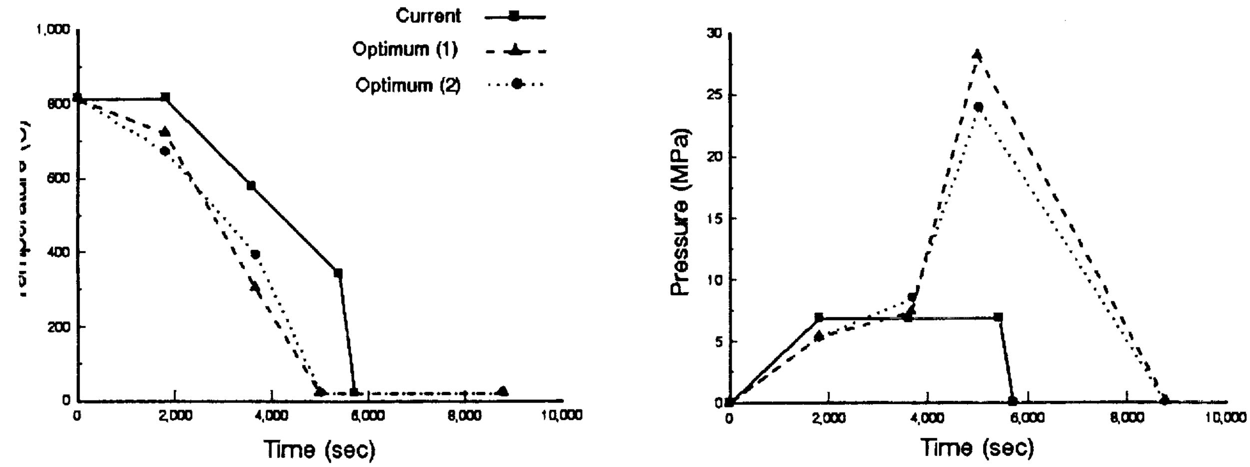
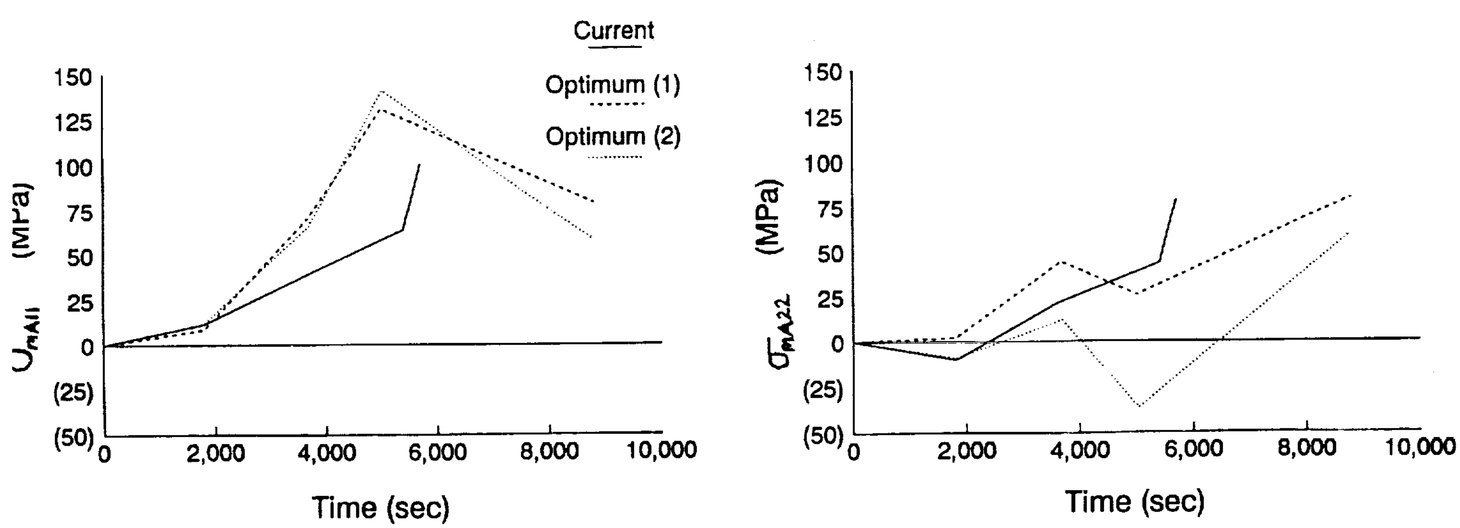


Figure 2. - Material Microregions in a Representative MMC Cell



(a) (b)

Figure 3. - Optimum and Current Cool-Down Phases for P100/Copper



(a) Longitudinal Stress (b) Transverse Stress

Figure 4. - Matrix Microstresses Developed During the Cool-Down Phase of P100/Copper

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16. Abstract

A method is presented to minimize the residual matrix stresses in metal matrix composites. Fabrication parameters such as temperature and consolidation pressure are optimized concurrently with the characteristics (i.e., modulus, coefficient of thermal expansion, strength, and interphase thickness) of a fiber-matrix interphase. By including the interphase properties in the optimization of the fabrication process, lower residual stresses are achievable. Results for a ultra-high modulus graphite (P100)/copper composite show a reduction of 21% for the maximum matrix microstress when optimizing the fabrication process alone. Concurrent optimization of the fabrication process and interphase properties show a 41% decrease in the maximum microstress. Therefore, this optimization method demonstrates the capability of reducing residual microstresses by altering the temperature and consolidation pressure histories and tailoring the interphase properties for an improved composite material. In addition, the results indicate that the consolidation pressures are the most important fabrication parameters, and the coefficient of thermal expansion is the most critical interphase property.

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